

CCS News Bytes

LALP-06-059

January-February-March 2006



Coyote has moved into Room 341 of the Laboratory Data Communications Center.

Coyote Arrives in LDCC, Joins Turquoise Network

"Coyote," the newest addition to the list of resources on Institutional Computing's Turquoise Network, began arriving at the Los Alamos National Laboratory Data Communications Center (the LDCC) in Technical Area 3 in late February.

Two of its major pieces were in place in Room 341 of the LDCC by the close of business on March 1—surrounded by a swarm of people starting to connect the necessary wires to make Coyote available to users.

Andy White, director of Institutional Computing, said he expected all of the parts to be in place by the end of March. "It's difficult to put together machines of this complexity," he said, but he added, "We hope to be up and running production science in early May."

By March 20, all of the pieces had arrived, and Bob Tomlinson, project leader for installation of Coyote, said it is "by far the largest *open* computer that we have in Los Alamos." He described it as "a huge new resource for doing open research." Acceptance tests and several other steps must be completed before Coyote is ready for use, but Tomlinson noted that Harvey Wasserman of High Performance Computing

Systems (CCN-7) was already offering classes on how to use the machine.

Ken Koch, scientific advisor on computing in the CCS Division Office, said Coyote "will provide vast opportunity for computing in the open for a breadth of unclassified areas." He noted that, "The machine is actually a cluster of clusters," and he said, "It's predominantly expected to host multiple jobs running independently on each subcluster—but it can also be configured into one large machine."

Richard Rivera, site-prep engineer on the project, said that the system weighs 84,828 pounds. It requires 1,556 square feet of space and 194 miles of networking cable. Its total power consumption in watts is 493,417; it produces 1,683,539 BTUs of heat per hour; it requires 168.4 tons of cooling to counter that heat; and it requires 95,341 cubic feet of air per minute to cool it.

The Laboratory is leasing the new 2804-processor, 1402-node computer system from Linux Networx, a company with corporate headquarters in Bluffdale, Utah, (just south of Salt Lake City), that sells supercomputers built from clusters of interconnected Linux servers. The lease—for a period of 36 months—will cost an estimated \$7.8 million.

(Please see Coyote, page 2.)

Division's Future Explained

The organizational future of what is now the Computer and Computational Sciences Division (CCS) became clear during a series of all-hands meetings held in March. Here it is, in a nutshell:

When Los Alamos National Security, LLS, (LANS), takes over management of Los Alamos National Laboratory on June 1, what is now CCS will be joined by D-1 (now the Statistical Sciences Group in the Decision Applications Division) to form a new division called the "Computer, Computational, and Statistical Science Division" (called CS for short). Stephen R. Lee, now deputy division leader in CCS, has been asked to serve as the CS Division director.

(Please see Future, page 2.)

Future (Cont'd from p.1)

CS will be within the new "Theory, Simulation, and Computation Directorate (TSC)," to be headed by Alan R. Bishop, currently head of the Theoretical Division (T Division). The other divisions within this new directorate will be T Division; a new "High Performance Computing Division" composed of Computing, Communications and Networking (CCN) 7, 8, 9, 12, and 18; and a new "Computing, Telecom, and Networks Division," composed of five groups that are now CCN 1, 2, 3, 4, and 5.

TSC will be within the new "Science, Technology, and Engineering Principal Associate Directorate (STE)." Terry Wallace, now associate director for strategic research, has been named the acting associate director of this new principal associate directorate. He is also a candidate for the permanent position.

William J. Feiereisen, now CCS Division leader, will move to Wallace's office, where he will coordinate high-performance computing. He will also have a role in Bishop's office.

In a March 21 e-mail to all employees of the division, Feiereisen said, "...Terry and Alan have asked me to join both of them on June 1st in an appointment between STE and TSC to develop and implement strategy for science-based prediction. There are three aspects to this. With the change in contract there is a unique opportunity to restore and increase our leadership in high performance computing; jointly for the weapons program, for the threat reduction community, and for our unclassified basic science. There continues to be a need for greater understanding of basic computer science to all three of the Lab missions and a watchdog and advocate for these opportunities. And there needs to be someone who consciously looks for connections between our awesome experimental and computational facilities to make us more than our competition at other labs.

"Many of you have heard us advocate for years that there should be an associate director for computing. The STE principal directorate will actually be more than this. This will be an opportunity to accomplish those things that a directorate for computing would have accomplished in our previous narrower view, but now expanded to include experiment also.

"I have greatly enjoyed my time in CCS and have learned a lot from all of the world-class people in this division. I thank you for your support and now ask for your help in making this broader vision a reality in our new organization. I will still be close by and actually hope to spend more time working with you representing your work to the Lab and the outside world in pursuit of the goals above.

"CCS is a strong division and will be central to the success of the new directorate. I look forward to supporting the goals of the division under Stephen's leadership from my new position. If any of you have strategic thoughts or ideas on science-based prediction and the role of CCS or the new directorate, I encourage you to share them with me."

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Coyote (Cont'd from p.1)

Leasing is a relatively new practice for the Laboratory, but White noted that it has major advantages. The Laboratory will pay nothing until Coyote is up and running, and it will be easy for the Laboratory to maintain discipline once Coyote is operating. LANL can always give Coyote back.

White described Linux Networkx as a successful, well-respected firm. "Pink," which has been part of the Institutional Computing lineup of resources for some time, is also a Linux Networkx computer, he said, as are several other machines in use for open and classified computing at the Laboratory. Pink uses CCS-1's "Science Appliance" software stack, and the new computer will too.

The new chief executive of Linux Networkx, appointed in June 2005, is no stranger to the Laboratory. Several years ago, Robert "Bo" Ewald was the leader of LANL's computing division. Before joining Linux Networkx, he was the president of Human Resource Solutions, and he is also a former chief operating officer of both Cray and Silicon Graphics.

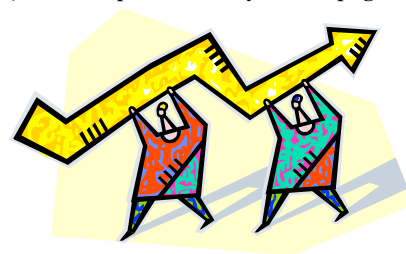
White said that when Institutional Computing was looking for new resources, it evaluated machines on "how much science over the year the machine would produce." Coyote was not necessarily the fastest machine available, he said. "It's about speed—and it's about the number of problems you can fit on the machine at the same time."

Institutional Computing encourages every scientist and engineer at the Laboratory to submit proposals for the use of its resources. Fifty-one proposals—totaling a little less than 42 million central processing unit hours—are already queued up, waiting for Coyote.

Asked to list a few of the proposals that will benefit from using Coyote, White mentioned five.

- Bette Korber of Theoretical Biology and Biophysics (T-10) is looking at HIV evolution and vaccine design.
- Joseph Carlson of Nuclear Physics (T-16) is doing research on supernovas.
- Beth Wingate of Continuum Dynamics (CCS-2) is studying mixing in the oceans.
- Steven Valone, Structure/Property Relations (MST-8), is studying irradiated metals and alloys.
- And David Steedman of Systems Engineering and Integration (D-3) is doing research involving deeply buried targets.

(For more photos of Coyote, see page 3.)



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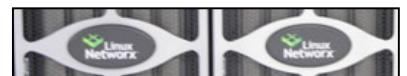


COYOTE ARRIVES *AND INSTALLATION BEGINS*

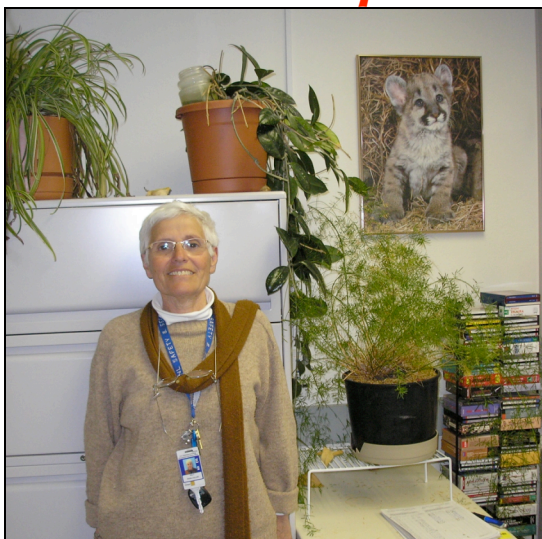
Robert Cummins of Linux Networkx, below, and two men from Santa Fe Services (at bottom) work on the thousands of tasks necessary to install the largest open computer at Los Alamos National Laboratory.



PHOTOS BY ANDY WHITE
AND CHARMIAN SCHALLER



Meet Our New People



Nely Padial-Collins

Nely Padial-Collins is a new staff member in Continuum Dynamics (CCS-2), but she is not new to Los Alamos National Laboratory (LANL). She has a wealth of prior experience here.

Padial-Collins, who joined CCS-2 on October 1, is a physicist who holds a master's degree in solid-state physics and a doctorate in atomic and molecular physics from the State University of Campinas in Brazil. Her past education also includes two postdoctoral appointments—one at the Joint Institute for Laboratory Astrophysics at the University of Colorado, and one at Rice University, where she specialized in atomic and molecular physics.

While she was at Rice, she worked simultaneously as a consultant for the Theoretical Chemistry and Molecular Physics Group at the Laboratory (T-12). She then became a staff member in the Computational Fluid Dynamics Group (T-3), where she worked for 17 years, specializing in hydrodynamics.

At T-3, she worked with two main codes: CFDLib, the computational hydrodynamics library, and CartaBlanca, a high-efficiency, object-oriented, general-purpose computer simulation environment in Java.

In 2005, she was part of a group that won an R&D 100 award for CartaBlanca. (The project leader was Brian VanderHeyden, and the other project members, besides Padial-Collins, were Duan Zhang, Qisu Zou, Giovanni Lapenta, and Stefano Markidis.)

Asked what attracted her to CCS-2, she said, "I knew some people in this group. I thought they were doing very nice work—and I thought I could contribute."

She is now working on the Crestone project, implementing a turbulence model in the RAGE code, and trying to improve performance of the code itself.

Padial-Collins' family life has a notable international flavor. She was born in Brazil, but her mother was originally from Italy, and her father was from Spain. After earning her doctorate, she worked in Brazil at the State University of Campinas in solid state and atomic and molecular physics.

She met her husband, Lee Collins, while both of them were pursuing postdoctoral studies in Boulder, Colorado, where they had the same mentor. Lee Collins was already working at LANL, and after they were married in 1981, she came to Los Alamos with him. He is now a Laboratory Fellow as well as a staff member in the Atomic and Optical Theory Group (T-4).

"I love New Mexico," she commented.

Their son, Gustavo, is an electrical engineer working in Atlanta, Georgia. He and his wife, Graziela, have a five-year-old son, Stefan.

Padial-Collins has two hobbies: gardening and opera.

Her office is filled with large, healthy, green plants, a small representation of her garden.

She said that living so near the Santa Fe Opera "is a treat for us," but she and her husband have also attended opera performances in other countries—Italy, Russia, and England. They go to the Metropolitan Opera in New York City every year.

Photographs in her office reveal a love of family—and a great affection for two large cats and two small ones.

Andrey Mirtchovski joined the Advanced Computing Laboratory (CCS-1) Cluster Research Team in October 2005.

Mirtchovski was born in Plovdiv, Bulgaria, and graduated from the "Model High School of Mathematics" in his hometown. Subsequently, he was granted an International Student Entrance Scholarship that enabled him to attend the University of Saskatchewan in Saskatoon, Canada. In conjunction with his studies there, he explored "Plan 9 from Bell Labs," an operating system created by the same people

(Please see People, page 5.)



Gina Fisk, new OCSR

Fisk Becomes Division OCSR

Gina Fisk, a veteran of 10 years at Los Alamos National Laboratory, became the organizational computer security representative (OCSR) for the Computer and Computational Sciences Division (CCS) in January. She has moved from her old office in the Advanced Computing Laboratory to a new one—Room 380 in the Laboratory Data Communications Center.

She now serves as the cyber-security advisor to the CCS Division director. She is also the CCS information system security officer (ISSO).

Her work involves doing operational security for the division, handling all cyber-security incidents that arise, and working with all foreign visitors to the division. She will soon be an authorized derivative classifier (ADC) as well. “I work as a liaison between the (CCS) Division and S Division,” she said in summary.

In addition to her security work, she serves as the division liaison for students, and she is in charge of “taking royalty money and turning it into scholarships.”

She said she spent about a week in training for her new OCSR position.

She has already had to deal with several issues.

One special task she has undertaken is to get the division’s security plan recertified. She explained that once a division develops a security plan, the plan must be approved and reviewed to make sure that the division’s operations are actually in accordance with the plan. Subsequently, the plan must be recertified every three years.

Asked what message she would like to share with employees in CCS, she said, “I guess the most important thing is to tell (the appropriate) people when things happen.” CCS employees who detect what

might be a cyber-security incident should inform their group leaders or come straight to Fisk. Her telephone number is 667-6769, and her e-mail address is gina@lanl.gov.

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People (Cont’d from p.4)

who created UNIX. He described it, in a recent interview, as “a small, very cleanly designed and clearly executed system ... a joy for a programmer to work with.”

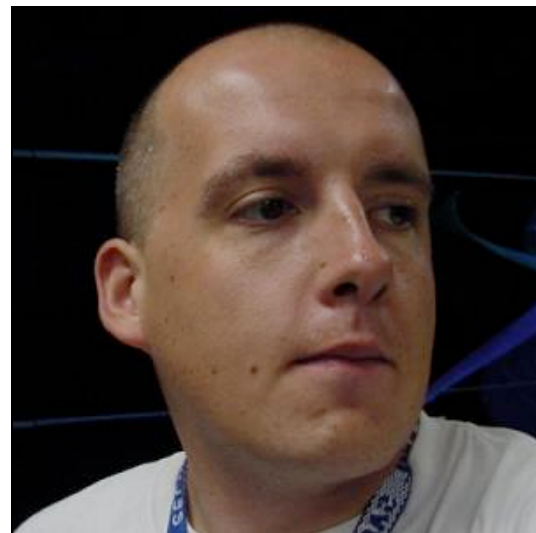
After earning a bachelor’s degree in computer science (with honors), he spent six months as a student employee at CCS-1 in Los Alamos, working on Linux Bios and Plan 9 projects.

He then returned to Canada and earned a master-of-science degree in computer science at the University of Calgary.

Last fall, he returned to Los Alamos National Laboratory as a technical staff member. Asked what brought him back to the Laboratory, he said that his experiences here as a student convinced him that, “It was just a fantastic place to work—completely different from industry.” He said he was also attracted to CCS-1 by the work the group is doing. He described the group as “the best collection of systems people that exists.”

He is now working on XCPU, a system for starting remote jobs on clusters and grids.

Asked about his life away from the Laboratory, he said he is married and living in Los Alamos. He enjoys skiing, hiking, and mountain biking. His wife, Petya, also Bulgarian, holds a master’s degree in education.



Andrey Mirtchovski

(Please see More People, p.6.)

More People (Cont'd from p.5.)



Galen Shipman

Galen Shipman, originally from Albuquerque, joined the Advanced Computing Laboratory (CCS-1) in January as a technical staff member.

Shipman earned an undergraduate degree in finance from the University of New Mexico (UNM)—and then shifted gears and earned a master's degree in computer science from UNM in December 2005. His advisor was Barney McCabe, a professor who runs the high-performance computing center at UNM.

During the summer of 2005, Shipman worked as a graduate student on the Applications Communication and Performance Research Team in CCS-1, contributing to Open MPI by implementing Infiniband support and contributing to the general communication architecture.

At UNM, his research included: 1) providing scalable Infiniband support to high-performance computing systems by utilizing features of the Infiniband architecture previously unused in HPC; 2) quantifying the costs of user-level reliability, which included adding a Raw Ethernet Path to LA-MPI and adding profiling code to the Linux TCP/IP stack; and 3) designing a user-level reliability protocol, which will allow a user to make the performance/reliability tradeoff appropriate for the environment.

One of Shipman's long-term goals is to earn "a doctorate in computer science doing systems research."

He is married and living in Albuquerque. He commutes to work by plane. "It's not bad," he said. "It's better than driving." His wife, Marie, is a satellite software engineer for ASRC Aerospace in Albuquerque.

His hobbies are skiing and flying. He is working on getting a pilot's license.

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In Case You Missed It....

Because of the conversion of an emergency exit on the second floor, south side of SM-200 to an entry point with a palm reader, it is now possible for people with L and Q clearances to go from the Advanced Computing Laboratory or Building 508 into Building 200 without going to the outside palm gate or going through three badge readers in T Division. The same stairwell also makes it possible to walk between the upper and lower stories of Building 200 without going outside. And, by providing easier access to Building 200, it provides an easier route to the Laboratory Data Communications Center (the LDCC). Deputy Division Leader Stephen Lee thanked **Chief of Staff Erma Pearson** for "keeping after this and getting it done," adding, "Nice work that benefits us all!"

CCS Division's participation in the Laboratory Directed Research and Development (LDRD) proposal-assessment process is notable this year. **Don Hush**, CCS-3, division point of contact for LDRD, said that CCS has one member on the LDRD-Directed Research Review Committee (**Ron Minnich** of CCS-1), and 11 members on various LDRD-Exploratory Research committees. Two of the ER committees are chaired by CCS staff members: the Computer and Information Science Committee is chaired by **Kei Davis** (CCS-3), and the Mathematics and Computational Science Committee is chaired by **Michael Hall** (CCS-2).

Five CCS-2 scientists—**Scott Elliot, Matthew Hecht, Balu Nadiga, Mark Petersen, and Beth Wingate**—attended the 13th Ocean Sciences Meeting in Hawaii in February. The American Geophysical Union, the American Society of Limnology and Oceanography, and The Oceanography Society were the major sponsors of the meeting. Hecht chaired an all-day session on "Eddy-Resolving Ocean Modeling" that drew an overflow crowd. His presentation was on "Sensitivity of North Atlantic Circulation to Topography and Sub-Gridscale Parameterization." Nadiga presented his work on the formation of alternating zonal jets in the world oceans. Petersen (whose co-authors were Hecht, Wingate, and Darryl Holm, also of CCS-2) presented a poster entitled "The LANS-Alpha Model of Sub-Gridscale Turbulence in the POP Ocean Model." Wingate gave a talk entitled "On the Existence of Potential Enstrophy Inertial Ranges." And Elliot presented a poster on "Carbon Monoxide in the Parallel Ocean Program."

HPCwire.com, a web-based newsletter specializing in stories on high-performance computing, ran an extensive story in March on the Performance and Architecture Laboratory (PAL), headed by **CCS-3 Group Leader Adolfo Hoisie**. The article spoke of PAL's ability to analyze very large-scale machines to determine whether they are performing up to their potential.

(Please see In Case, page 7.)

In Case (Cont'd from p.6.)

The article quoted **CCS Division Leader William Feiereisen** as saying that PAL's models are overall predictors of how the whole system performs—hardware, software, and algorithm characteristics.

The San Francisco Chronicle recently ran a story on the importance of improving mathematics education in the United States. In the middle of the article, the magazine described the work of **Cliff Joslyn, CCS-3**, as one of several examples of just how important mathematics can be—notably in the fight against terrorism. The article was listed on the Laboratory's home page.

The Computer and Computational Sciences Division (CCS) lost an old friend January 20 when **Doug Kothe** accepted an offer to become director of science in the National Center for Computational Sciences at Oak Ridge National Laboratory. Most recently, Kothe had been deputy program director for theoretical and computational programs in the LANL associate directorate for Nuclear Weapons Programs. Before that, he had been acting deputy division leader of CCS. In announcing Kothe's departure, James S. Peery, principal deputy associate director for Nuclear Weapons Programs, said, "...I believe we have all greatly benefited from Doug's vision, energy, and concepts put into defining the future National Nuclear Security Administration (NNSA) Advanced Simulation and Computing (ASC) program."

On January 16, **Wu-chun Feng** of CCS-1 announced that after seven years at LANL, he was leaving Los Alamos for a career in the Department of Computer Science at Virginia Tech.

He sent out a CCS-all e-mail message thanking "all the folks who made my work possible..." He said, "Specifically, a lot of what I managed to accomplish here at LANL can be attributed directly to the staff and students that I have had the privilege to work with as well as to management for their unwavering support of my work. Nowhere else in the world would I have been able to do what I have done over the past seven years."

His new address is: Professor Wu-chun Feng, Mail Code 0106, Department of Computer

Science, Virginia Tech, Blacksburg, Virginia, 24061.

A new book, "Computational Complexity and Statistical Physics," edited by **Allon Percus** (CCS-3), and **Gabriel Istrate** (CCS-5)—along with Cristopher Moore of the University of New Mexico—was released in February by Oxford University Press.

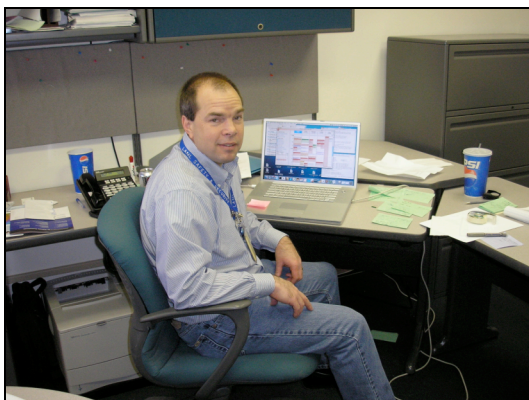
The book, aimed at a broad range of readers, is intended to serve as a standard reference to statistical physics methods in computer science theory, focusing on phase transitions in combinatorial problems.

Belinda Edwards, deployed human resources generalist assigned in CCS, was among artists honored in an art exhibition in the New Mexico Governor's Office during Black History Month. A news release from the governor's office spoke of her "exceptional pen and ink drawings."

Security Tips

If you have not yet gotten a personal identification number (PIN) at the Badge Office, you should do it immediately. In the next few days, a change will go into effect that will require *pedestrians* to enter a PIN to use Post 411 (the Back Gate), the rear entrance to the Administration Building. (The vehicle gate will not be automated.) On April 3, the PIN requirement will go into effect at Post 414 (the "Chicken Shack" at the Laboratory Data Communications Center) and at Post 336 (SM-39, the Shops). And on May 1, the Laboratory will begin requiring a PIN for those who want to use Post 311 (the Chemistry and Metallurgy Research Facility entrance/east).

On April 1, the National Nuclear Security Administration (NNSA) will begin requiring employees at Los Alamos National Laboratory (and all other NNSA facilities) to submit all "Questionnaires for National Security Positions (QNSPs)" electronically. Anyone using a QNSP for an initial clearance request, upgrade, reinstatement, or reinvestigation will have to complete and submit the QNSP on a secure federal website maintained by the Office of Personnel Management. The change is intended to increase efficiency. For full details, read (and retain) the all-employees bulletin sent out by e-mail on March 16 at 10:22 a.m.



Richard Graham

Graham Appointed as Acting CCS-1 Leader

Richard Graham, who was appointed in February as the acting director of the Advanced Computing Laboratory (CCS-1), has been at Los Alamos National Laboratory (LANL) for seven years and brings a wealth of experience to the position.

In an e-mail announcement of Graham's appointment, Computer and Computational Sciences (CCS) Division Leader William J. Feiereisen said, "Rich is an excellent addition to the management of CCS, and I am very happy that he has accepted this position." Feiereisen added, "Stephen Lee has been the acting group leader since late September and has helped out greatly in the organization and management of the group. I'm very pleased with his tenure as acting group leader and what he has accomplished. He is coming back to the Division Office and will again take up his duties as deputy division leader. Thank you, Stephen! Welcome, Rich!"

Graham was still moving in when he granted an interview on March 21. Asked what attracted him to his new job, he said that CCS-1 is "one of the strongest applied computer research organizations in the world. Period." He noted that CCS-1 provides the software that runs on large Advanced Simulation and Computing Linux systems at the Laboratory "day in and day out."

CCS, he said, is "a very strong research and development organization. The challenge is to figure out how we can build on this and become even stronger."

At present, Graham is doing double duty at the Laboratory. He is also the Computer Systems and Software Environment (ASC) Program manager, and, with the support of Brett Kettering in the Computing, Communications and Networking (CCN) Division, he will retain this position—in addition to heading CCS-1—during the transition to a new Laboratory contract.

In a way, Graham has come full circle at the Laboratory by accepting a leadership post at CCS-1. He joined CCS-1 in 1999 when he first came to Los Alamos as a technical staff member. As team leader for the Resilient Technologies Team, he started the

LA-MPI project, and he was one of the founders of the Open MPI collaboration.

When he came to Los Alamos, he brought to the Laboratory a background that was both varied and interesting.

He grew up in Israel, where his parents were missionaries. He earned a bachelor of science degree in chemistry from Seattle Pacific University; did one year of graduate work at the University of Washington; and then transferred to Texas A&M, where he earned a doctorate in theoretical chemistry.

Subsequently, he did postdoctoral work in theoretical chemistry at the James Franck Institute at the University of Chicago.

When he left Chicago, he joined Cray Inc. in Eagan, Minnesota, where he spent four years developing and maintaining a computational chemistry resource for the pharmaceutical industry. He then moved to Pittsburgh, Pennsylvania, where he worked for Cray/SGI at the Pittsburgh Supercomputing Center (PSC), one of Cray/SGI's customers, running Cray's Parallel Applications Technology Program team at the PSC.

His next move was to SGI, where he started as an applications analyst and ended up running SGI's Applications and Software on-site team at LANL, working on Bluemountain.

Finally, he became a Laboratory employee. Today, he and his wife, Ruth, live in White Rock. They have four children: sons Nathan, 19; Daniel, 15; and Jonathan, 13; and a daughter, Tali, 7.

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Java City, on the east-side ground floor of the Laboratory Data Communications Center, is a great new addition for those who sometimes want something to drink but don't want to walk for miles or struggle with a machine. The little shop offers espresso drinks, hot beverages, and even iced specialties.